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**CODEN: IAASCA** **ORIGINAL ARTICLE**

# Structural Investigations and Cation Distribution of Zn Substituted $MnFe_2O_4$ Spinel Ferrite Nanoparticles

**V. D. Murumkar**
Department of Physics, Vivekanand Arts, Sardar Dalipsingh Commerce and Science College, Aurangabad

**ABSTRACT**
*The structural properties of nanocrystalline manganese and zinc substituted manganese spinel ferrites are presented here. The structural properties of Mn-Zn spinel ferrite was studied by X-ray diffraction technique. The recorded XRD patterns for Mn-Zn spinel ferrite showed the cubic spinel structure. The XRD data was used to obtain the structural parameters such as crystallite size, lattice parameter, X-ray density etc. Moreover the cation distribution was done by using XRD data.*
***Keywords:*** *Mn-Zn spinel ferrite, XRD, Lattice parameter, Cation distribution*

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## INTRODUCTION

The magnetic materials have played a great number of crucial roles in the daily life because of their useful properties. Among the magnetic materials, the polycrystalline ferrites have been paid special attention due to their chemical stability as well as their excellent combination of electrical and magnetic properties. On the basis of their high electrical resistivity, low eddy current and dielectric losses, high saturation magnetization and high permeability these materials have been employed in many technological areas [1].

The crystal structure of ferrites is of different types as cubic spinel, cubic garnet and hexagonal. On the basis of crystal structure ferrites are classified into three groups, namely spinel ferrite, garnet and hexagonal ferrite [2]. Among these ferrites, spinel ferrites are the most important and widely studied by number of researchers. Spinel ferrite with cubic spinel structure possess two interstitial sites namely, tetrahedral (A) site and octahedral [B] site. The metal cations reside at tetrahedral and octahedral sites depending upon their ionic radii and site preference energy [3].

## RESULTS AND DISCUSSION

X-ray diffraction studies of a material give important information about the structure and phase of the material. Various structural parameters such as lattice constant, particle size, X-ray density, porosity and cation distribution can be calculated from the studies of X-ray diffraction. Zinc substituted manganese ferrite samples synthesized by sol-gel technique were characterized by X-ray diffraction technique in the 2θ range of 20-80 degree with Cu-Kα radiation of wavelength λ = 1.5406 Å. The X-ray diffraction patterns were recorded at room temperature and presented in figure 1.

### Indexing of planes:

The XRD patterns recorded at room temperature are shown in figure 1. All the reflections present in the XRD patterns were indexed by using Bragg's law. The presence of planes (220), (311), (400), (422), (511) and (440) in the XRD pattern reveals the cubic spinel structure of the samples [4]. It is also evident that all the reflection peaks are intense and sharp. No impurity peaks were observed; so, the samples are single phase in nature.

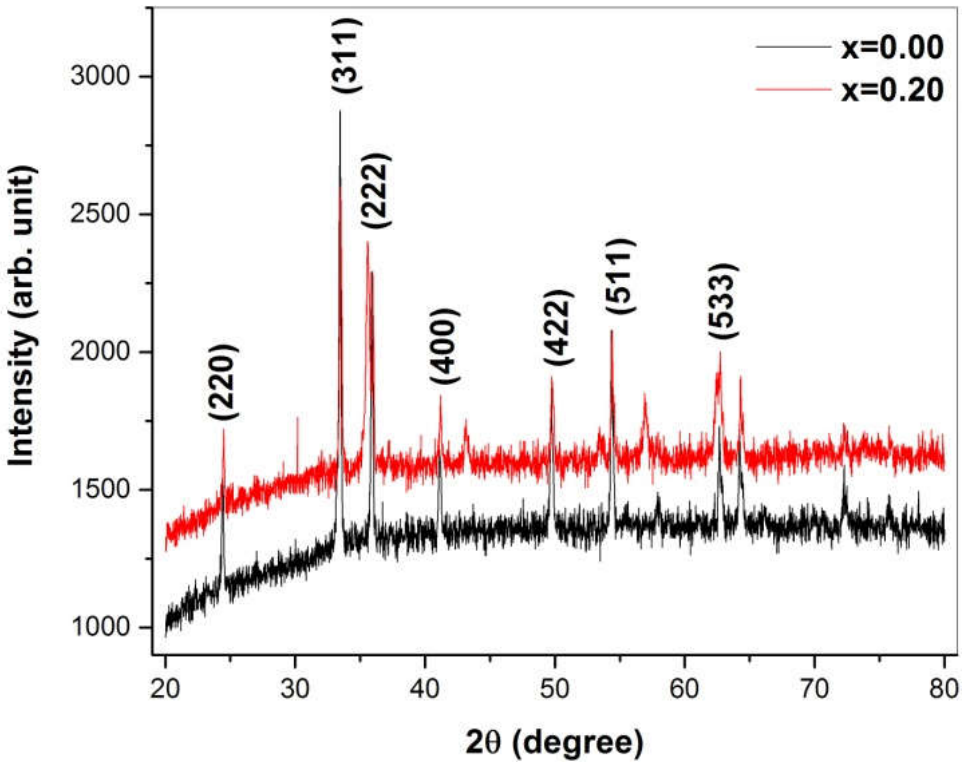


Figure 1: XRD patterns for $Mn_{1-x}Zn_xFe_2O_4$ with x=0.00 and x=0.20

**Lattice parameter (a):**

The lattice parameter (a) values of nanocrystalline zinc substituted manganese spinel ferrite samples were calculated using standard relation,

$a = d\sqrt{(h^2+k^2+l^2)}$

where, (d) is inter-planar spacing and (h k l) is Miller Indices.

The obtained values of the lattice parameter show gradual decrease with the substitution of zinc for manganese in the present ferrite system. The decrease in the lattice parameter is obvious and is attributed to the larger ionic radius of the manganese (0.91Å) than that of the zinc (0.82Å). The behaviour of lattice parameter of the present samples is analogous to the literature reports on the zinc substituted spinel ferrite system [5].

**Crystallite size (t):**

The crystallite size of Mn-Zn ferrite was calculated by using peak broadening of the most intense (311) peak and using the Debye-Scherrer's relation for small and uniform sized cubic crystals mentioned below [8],

$$t = \frac{0.9\lambda}{\beta \cos\theta}$$

where, λ is wavelength of the Cu-Kα radiation, β is the full width of the half maximum (FWHM) of the XRD peak and θ is Bragg's angle. The obtained values of the crystallite size are presented in table 1. From the table 1 it is seen that the crystallite size of manganese spinel ferrite decreases.

**Physical parameters:**

The physical parameters such as X-ray density ($d_X$), bulk density ($d_B$) and the porosity (P) were also calculated for each sample. The X-ray density ($d_X$) was calculated by using the relation;

$$d_x = \frac{Z \times M}{V \times N_A} \text{ gm/cm}^3$$

where, (Z) is the number of molecules per formula unit (Z = 8 for spinel system), (M) is molecular weight of the sample, ($V = a^3$) is the unit cell volume, ($N_A$) is the Avogadro's number.

To calculate the bulk density the pellets were used and the formula given as;

$$d_b = \frac{m}{V} \quad \text{gm/cm}^3$$

where, (m) is the mass of pellet, (V) is the volume of pellet. The bulk density was found to be decreasing with increase in zinc content x.
The porosity of the materials can be obtained from the values of X-ray density and bulk density as given by the equation:

$$p = 1 - \frac{d_b}{d_x}$$

The obtained values of these physical parameters are tabulated in table 1. From the table 1 it is observed that the X-ray density and bulk density decreases with the zinc. The percentage porosity calculated from the values of X-ray and bulk density values goes on increasing.

Table 1: Crystallite size (t), lattice parameter (a), X-ray density ($d_x$), and Bulk density ($d_B$)

| Comp. x | T (nm) | A (Å) | $d_x$ (gm/cm$^3$) | $d_B$ (gm/cm$^3$) | P (%) | Cation distribution |
|---|---|---|---|---|---|---|
| X=0.00 | 33 | 8.4025 | 5.221 | 4.223 | 19 | $(Zn_{0.2}Fe_{0.8})$ $[Mn_{0.8}Fe_{1.2}]$ |
| X=0.20 | 27 | 8.3973 | 5.076 | 4.103 | 21 | $(Zn_{0.2}Fe_{0.6}Mn_{0.2})$ $[Mn_{0.8}Fe_{1.4}]$ |

**Cation distribution studies:**
The cation distribution in spinel ferrite can be obtained from the X-ray diffraction method using different methods as Bertaut [6], Furuhashi [7], and *R*-factor [8]. All these methods are based on a comparison between the diffraction intensities observed experimentally and those calculated for a large number of hypothetical crystal structures. In the present work, the Bertaut method based on X-ray diffraction was used to determine the cation distribution. This method selects a few pairs of reflections according to expression [9, 10].

$$\frac{I_{obs}^{hkl}}{I_{obs}^{h'k'l'}} = \frac{I_{cal}^{hkl}}{I_{cal}^{h'k'l'}}$$

where $I_{obs}^{hkl}$ and $I_{cal}^{hkl}$ are the observed and calculated intensities for reflection (h k l) respectively. If an agreement factor (R), is defined as

$$R = \left| \frac{I_{obs}^{hkl}}{I_{obs}^{h'k'l'}} - \frac{I_{cal}^{hkl}}{I_{cal}^{h'k'l'}} \right|$$

In this method, the small value of the agreement factor (R) is the indicator of the reliability of the results. The most suitable reflections for the cation distribution studies are (220), (400), and (422). Table 1 shows the estimated cation distribution for the present ferrites samples. It is observed from table 1 that the zinc ions in all the samples occupy tetrahedral (A) site, while the manganese ions found to be distributed on both the tetrahedral (A) site and octahedral [B] sites.

**CONCLUSION**
The cubic spinel structure of bare and zinc substituted manganese spinel ferrite was confirmed by XRD pattern. The obtained structural parameters as crystallite size, lattice parameter, X-ray density etc are in the reported range. The crystallite size and lattice parameter were found to decrease with zinc substitution. The cation distribution revealed that Mn occupy both tetrahedral as well as octahedral sites.

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